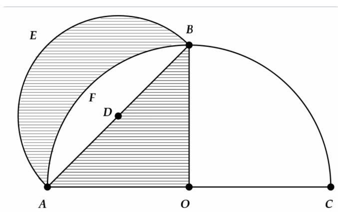
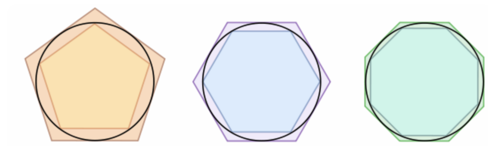
Ch 4.3 - 4.7 Numerical Integration

- Historically known as quadrature, Pythagoreans in ancient Greece computed the area of a region by finding a square that had the same area.
- Archimedes used the method of exhaustion as well, in contrast to the method of quadrature. (Wikipedia → Numerical Integration)

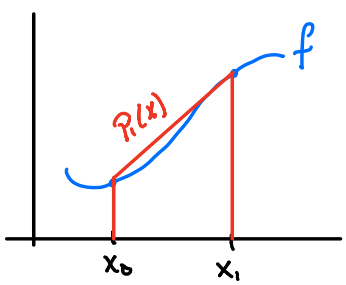


The lune of Hippocrates is the upper left shaded area. It has the same area as the lower right shaded triangle.



Archimedes used the method of exhaustion to compute the area inside a circle

As with numerical differentiation, we start with a Lagrange interpolating polynomial through our data points.



Degree 1 Case (Trapezoid rule)

$$f(x) = P_1(x) + E_1(x)$$

$$= \frac{(x-x_1)}{x_0-x_1} f(x_0) + \frac{x-x_0}{x_1-x_0} f(x_1) + \frac{f''(\xi(x))}{2!}(x-x_0)(x-x_1)$$

$$\therefore \int_{x_0}^{x_1} f(x)\,dx = f(x_0)\underbrace{\int_{x_0}^{x_1} \frac{x-x_1}{x_0-x_1}\,dx}_{C_0} + f(x_1)\underbrace{\int_{x_0}^{x_1} \frac{x-x_0}{x_1-x_0}\,dx}_{C_1} + \underbrace{\int_{x_0}^{x_1} \frac{f''(\xi(x))}{2!}(x-x_0)(x-x_1)\,dx}_{E_1(x)}$$

$$\cong f(x_0)C_0 + f(x_1)C_1 \quad \leftarrow \text{quadrature rule (formula)}$$

$$= \sum_{k=0}^{1} f(x_k)C_k$$

If $f(x)$ is a polynomial of degree 1 or less, then $f''(x) = 0$ and $E_1(x) = 0$.

Ch 4.3 Overview: Numerical Integration

The basic method involved in approximating $\int_a^b f(x)dx$ is called quadrature.

Typically we first select distinct nodes $\{x_0, x_1, \dots, x_n\}$ from $[a,b]$. Using the Lagrange interpolating polynomial,

$$f(x) = \sum_{k=0}^{n} f(x_k)L_k(x) + \frac{f^{(n+1)}(\xi(x))}{(n+1)!}\prod_{k=0}^{n}(x-x_k)$$

Thus

$$\int_a^b f(x)dx = \sum_{k=0}^{n} a_k f(x_k) + \frac{1}{(n+1)!}\int_a^b f^{(n+1)}(\xi(x))\prod_{k=0}^{n}(x-x_k)dx$$

where $a_k = \int_a^b L_k(x)dx$, $k=0,1,\dots,n$.

Quadrature Formula: $\int_a^b f(x)dx \cong \sum_{k=0}^{n} a_k f(x_k)$

Error Formula: $E(f) = \frac{1}{(n+1)!}\int_a^b f^{(n+1)}(\xi(x))\prod_{k=0}^{n}(x-x_k)dx$

We have

$$\int_a^b f(x)\,dx = \underbrace{\sum_{k=0}^{n} a_k f(x_k)}_{\text{Quadrature Formula}} + \underbrace{\frac{1}{(n+1)!}\int_a^b f^{(n+1)}(\xi(x))\prod_{k=0}^{n}(x-x_k)\,dx}_{\text{Error Formula } E(f)}$$

<u>Definition</u> The <u>degree of accuracy</u>, or <u>precision</u>, of a quadrature formula is the largest positive integer n for which the formula is exact for x^k, $k=0,1,2,\dots,n$.

Thus if a quadrature formula has precision n, then it is exact for all polynomials $p(x)$ of degree at most n.

Newton-Cotes formulas are a class of methods used for quadrature, and include the Trapezoid Rule and Simpson's Rule from Calculus.

Trapezoidal Rule:

$$\int_a^b f(x)\,dx = \frac{h}{2}[f(x_0) + f(x_1)] - \frac{h^3}{12} f''(\xi).$$

This is called the Trapezoidal rule because when f is a function with positive values, $\int_a^b f(x)\,dx$ is approximated by the area in a trapezoid, as shown in Figure 4.3.

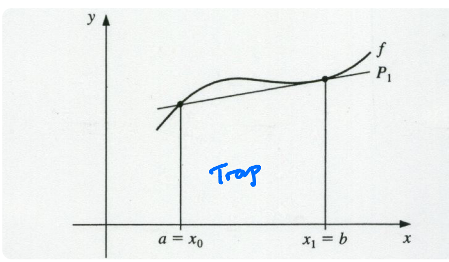
Degree of accuracy = 1

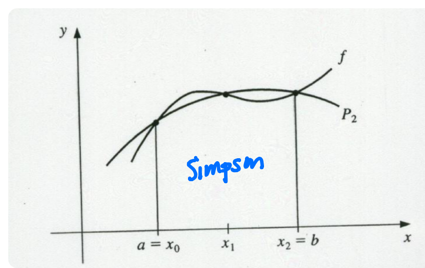
Simpson's Rule:

$$\int_{x_0}^{x_2} f(x)\,dx = \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] - \frac{h^5}{90} f^{(4)}(\xi).$$

Since the error term involves the fourth derivative of f, Simpson's rule gives exact results when applied to any polynomial of degree three or less.

Degree of accuracy = 3



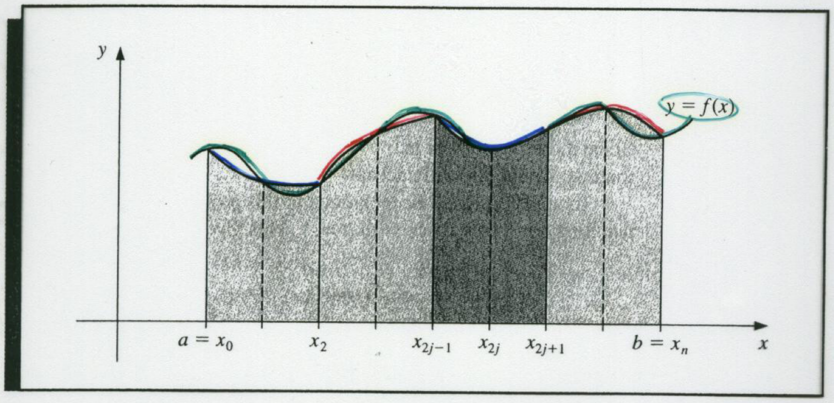


Theorem 4.4

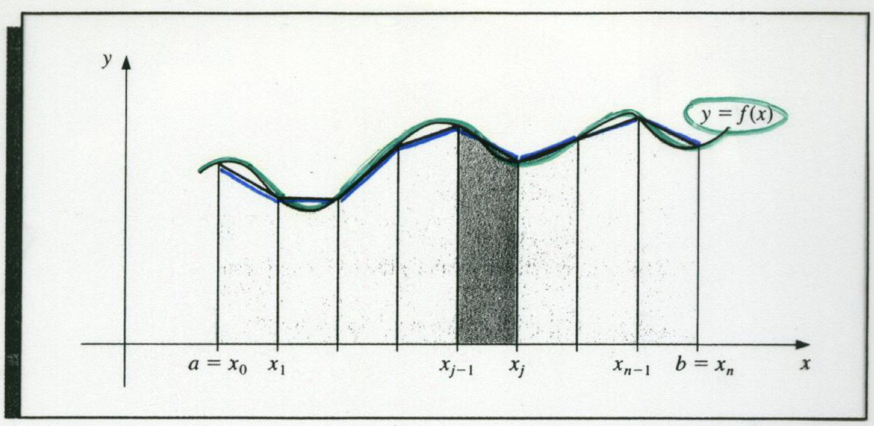
Let $f \in C^4[a, b]$, n be even, $h = (b - a)/n$, and $x_j = a + jh$, for each $j = 0, 1, \ldots, n$. There exists a $\mu \in (a, b)$ for which the **Composite Simpson's rule** for n subintervals can be written with its error term as

$$\int_a^b f(x)\,dx = \frac{h}{3}\left[f(a) + 2\sum_{j=1}^{(n/2)-1} f(x_{2j}) + 4\sum_{j=1}^{n/2} f(x_{2j-1}) + f(b)\right] - \frac{b-a}{180}h^4 f^{(4)}(\mu).$$

■



Theorem 4.5

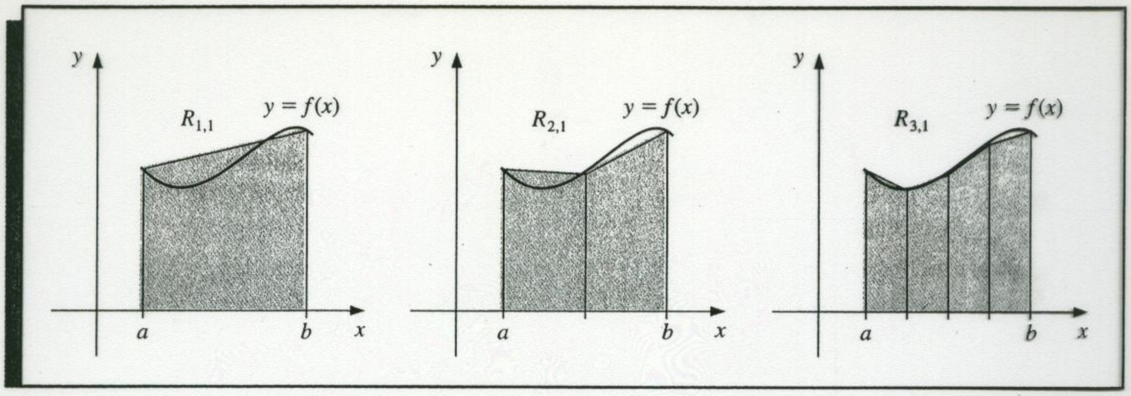


Let $f \in C^2[a, b]$, $h = (b - a)/n$, and $x_j = a + jh$, for each $j = 0, 1, \ldots, n$. There exists a $\mu \in (a, b)$ for which the **Composite Trapezoidal rule** for n subintervals can be written with its error term as

$$\int_a^b f(x)\,dx = \frac{h}{2}\left[f(a) + 2\sum_{j=1}^{n-1} f(x_j) + f(b)\right] - \frac{b-a}{12}h^2 f''(\mu).$$

■

Figure 4.10



$$R_{k,j} = R_{k,j-1} + \frac{R_{k,j-1} - R_{k-1,j-1}}{4^{j-1} - 1}.$$

The results that are generated from these formulas are shown in Table 4.9.

Table 4.9

$R_{1,1}$					
$R_{2,1}$	$R_{2,2}$				
$R_{3,1}$	$R_{3,2}$	$R_{3,3}$			
$R_{4,1}$	$R_{4,2}$	$R_{4,3}$	$R_{4,4}$		
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	
$R_{n,1}$	$R_{n,2}$	$R_{n,3}$	$R_{n,4}$	$\cdots$	$R_{n,n}$

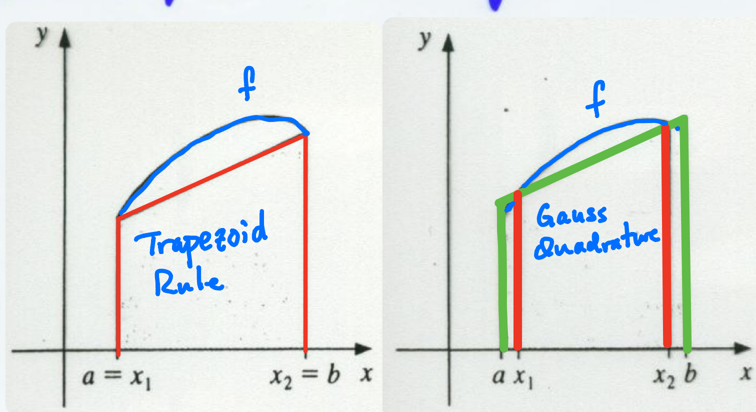
Ch 4.7: Gaussian Quadrature

Rather than choosing nodes in an equally spaced way, here we choose $x_1, x_2, \ldots, x_n$ in $[a,b]$ and coefficients $c_1, c_2, \ldots, c_n$ such that the expected error in the approximation

$$\int_a^b f(x)\,dx \cong \sum_{i=1}^{n} c_i f(x_i)$$

is minimized.

We assume that the best choice of these values is that which produces the exact result for the largest class of polynomials (greatest degree of precision).



The 2pt Gauss quadrature (on right) still uses a trapezoid over $[a,b]$, but the two nodes x_1, x_2 are not required to satisfy $x_1 = a$, $x_2 = b$.

Quadrature Formula:

$$\int_a^b f(x)\,dx \cong \sum_{i=1}^{n} c_i f(x_i)$$

The coefficients c_i, $i=1,\dots,n$ are arbitrary, and the nodes x_i, $i=1,\dots,n$ are restricted only by $x_i \in [a,b]$. This gives us $2n$ parameters to choose.

Since we want the quadrature formula to be exact for the largest class of polynomials, we consider

$$\mathbb{P}_{2n-1} = \{ p(x) : \deg p(x) \le 2n-1 \}$$

For example,

$$p(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_{2n-1} x^{2n-1}$$

is an element of $\mathbb{P}_{2n-1}$.

These polynomials have $2n$ coeffs, and will enable us to generate the equations we need to determine c_i & x_i.

Suppose $[a,b] = [-1,1]$. We seek exact formulas for

$$\int_{-1}^{1} 1\,dx, \quad \int_{-1}^{1} x\,dx, \quad \int_{-1}^{1} x^2\,dx, \quad \int_{-1}^{1} x^3\,dx$$

That is, we need c_1, c_2, x_1, x_2 such that

$$c_1 \cdot 1 + c_2 \cdot 1 = \int_{-1}^{1} 1\,dx = 2$$

$$c_1 \cdot x_1 + c_2 \cdot x_2 = \int_{-1}^{1} x\,dx = 0$$

$$c_1 \cdot x_1^2 + c_2 \cdot x_2^2 = \int_{-1}^{1} x^2\,dx = \frac{2}{3}$$

$$c_1 \cdot x_1^3 + c_2 \cdot x_2^3 = \int_{-1}^{1} x^3\,dx = 0$$

(Recall $\int_a^b f(x)\,dx \cong \sum_{i=1}^{n} c_i f(x_i)$)

Thus we have four equations in four unknowns, which can be solved using algebra.

① $c_1 + c_2 = 2 \Rightarrow c_1 = 2 - c_2$

② $c_1 x_1 + c_2 x_2 = 0$

$(2-c_2)x_1 + c_2 x_2 = 0 \Rightarrow x_2 = \left(\frac{c_2-2}{c_2}\right)x_1$

③ $c_1 x_1^2 + c_2 x_2^2 = \frac{2}{3}$

$\left[(2-c_2)x_1^2 + c_2\left(\frac{c_2-2}{c_2}\right)^2 x_1^2 = \frac{2}{3}\right]$

④ $c_1 x_1^3 + c_2 x_2^3 = 0$

$\left[(2-c_2)x_1^3 + c_2\left(\frac{c_2-2}{c_2}\right)^3 x_1^3 = 0\right]$

Thus the four equations in four unknowns reduces to two equations in two unknowns:

$$(2-c_2)x_1^2 + c_2\left(\frac{c_2-2}{c_2}\right)^2 x_1^2 = \frac{2}{3}$$

$$(2-c_2)x_1^3 + c_2\left(\frac{c_2-2}{c_2}\right)^3 x_1^3 = 0$$

Result: $c_1 = 1$, $c_2 = 1$, $x_1 = -\sqrt{3}/3$, $x_2 = \sqrt{3}/3$

Thus

$$\int_{-1}^{1} f(x)\,dx \cong 1 \cdot f(-\sqrt{3}/3) + 1 \cdot f(\sqrt{3}/3)$$

Two-Point Gaussian Quadrature:

$$\int_{-1}^{1} f(x)\,dx \cong 1 \cdot f\left(-\frac{\sqrt{3}}{3}\right) + 1 \cdot f\left(\frac{\sqrt{3}}{3}\right)$$

(on $[-1, 1]$)

<u>Example</u> $f(x) = 4x^3 + 3x^2 + 2x + 1$

<u>Exact</u>: $\int_{-1}^{1} (4x^3 + 3x^2 + 2x + 1)\,dx$

$$= (x^4 + x^3 + x^2 + x)\Big|_{-1}^{1}$$

$$= [1^4 + 1^3 + 1^2 + 1] - [(-1)^4 + (-1)^3 + (-1)^2 + (-1)]$$

$$= 1 + 1 + 1 + 1 = \underline{4}$$

<u>Quadrature</u>:

$$\int_{-1}^{1} f(x)\,dx \cong 1 \cdot f\left(-\frac{\sqrt{3}}{3}\right) + 1 \cdot f\left(+\frac{\sqrt{3}}{3}\right)$$

$$= 4\left(\frac{-\sqrt{3}}{3}\right)^3 + 3\left(\frac{-\sqrt{3}}{3}\right)^2 + 2\left(\frac{-\sqrt{3}}{3}\right) + 1$$

$$+ 4\left(\frac{\sqrt{3}}{3}\right)^3 + 3\left(\frac{\sqrt{3}}{3}\right)^2 + 2\left(\frac{\sqrt{3}}{3}\right) + 1$$

$$= \left[3\left(\frac{3}{9}\right) + 1\right] + \left[3\left(\frac{3}{9}\right) + 1\right] = \underline{4}$$

Two-Point Gaussian Quadrature on [-1,1]:

$$\int_{-1}^{1} f(x)\,dx \doteq 1\cdot f\left(-\frac{\sqrt{3}}{3}\right) + 1\cdot f\left(\frac{\sqrt{3}}{3}\right)$$

Example $f(x) = e^x$

Exact: $\int_{-1}^{1} e^x dx = e^x \Big|_{-1}^{1} = e^1 - e^{-1}$

$\doteq 2.35040238729$ (TI-86)

Quadrature

$$\int_{-1}^{1} f(x)dx = 1\cdot f\left(-\frac{\sqrt{3}}{3}\right) + 1\cdot f\left(\frac{\sqrt{3}}{3}\right)$$

$$= 1\cdot e^{-\sqrt{3}/3} + 1\cdot e^{\sqrt{3}/3}$$

$$\doteq 2.34269608791 \quad \text{(TI-86)}$$

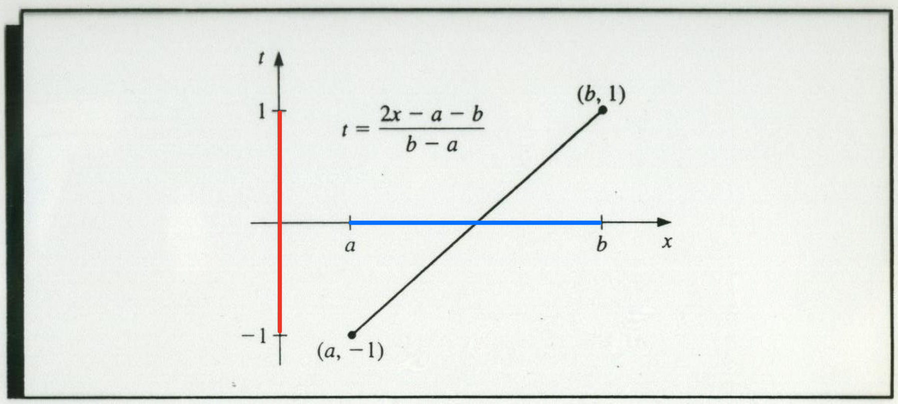
Relative Error: 0.00327871492

Legendre Polynomials → roots

Table 4.11

n	Roots $r_{n,i}$	Coefficients $c_{n,i}$
2	0.5773502692	1.0000000000
	−0.5773502692	1.0000000000
3	0.7745966692	0.5555555556
	0.0000000000	0.8888888889
	−0.7745966692	0.5555555556
4	0.8611363116	0.3478548451
	0.3399810436	0.6521451549
	−0.3399810436	0.6521451549
	−0.8611363116	0.3478548451
5	0.9061798459	0.2369268850
	0.5384693101	0.4786286705
	0.0000000000	0.5688888889
	−0.5384693101	0.4786286705
	−0.9061798459	0.2369268850

Figure 4.16



$$x = \frac{(b-a)t + (b+a)}{2}$$

$$dx = \frac{b-a}{2}\,dt$$

Recall from Theorem 4.7:

$$\int_{-1}^{1} p(x)\,dx = \sum_{k=1}^{n} c_k\, p(x_k), \quad \forall p \in \mathbb{P}_{2n-1}$$

where $$c_k = \int_{-1}^{1} \prod_{\substack{j=1 \\ j \neq k}}^{n} \frac{(x-x_j)}{(x_k-x_j)}\,dx$$

The coefficients $c_1, \ldots, c_n$, as well as the nodes $x_1, \ldots, x_n$, are extensively tabulated; hence there is no need to compute these ourselves.
See Table 4.11.
Also, for an integral $\int_a^b f(x)dx$ over $[a,b]$, we can transform to $[-1,1]$ using:

$$t = \frac{2x-a-b}{b-a}$$

That is, $[a,b] \xrightarrow{t} [-1,1]$
(Check this for $x=a$ & $x=b$.)
See Figure 4.16.

$$x = \frac{(b-a)t + (b+a)}{2}$$

$$dx = \frac{b-a}{2}\,dt$$

Thus, using the substitution

$$t = \frac{2x-a-b}{b-a}, \quad dt = \frac{2}{b-a}dx,$$

we have

$$\int_a^b f(x)dx = \int_{-1}^{1} f\left(\frac{(b-a)t+(b+a)}{2}\right) \cdot \frac{(b-a)}{2}dt$$

Example $\int_1^{1.5} e^{-x^2}dx$

Here, $t = \frac{2x-1-1.5}{1.5-1} = \frac{2x-2.5}{0.5} = 4x-5$

and hence $x = \frac{1}{4}(t+5)$, $dx = \frac{1}{4}dt$

Thus

$$\int_1^{1.5} e^{-x^2}dx = \frac{1}{4}\int_{-1}^{1} e^{-\frac{(t+5)^2}{16}}dt$$

See next page for Gaussian quadrature approximations.

$$\boxed{\begin{aligned} x &= \frac{(b-a)t+(b+a)}{2} \\ dx &= \frac{b-a}{2}dt \end{aligned}}$$

We have

$$\int_1^{1.5} e^{-x^2}\,dx = \frac{1}{4}\int_{-1}^{1} e^{-\frac{(t+5)^2}{16}}\,dt$$

Gaussian Quadrature (use Table 4.11)

n=2

$$\int_1^{1.5} e^{-x^2}\,dx \cong \frac{1}{4}\left[e^{-\frac{(5+0.5773502692)^2}{16}} + e^{-\frac{(5-0.5773502692)^2}{16}}\right] = 0.1094003$$

n=3

$$\int_1^{1.5} e^{-x^2}\,dx \cong \frac{1}{4}\Big[(0.5555555556)e^{-(5+0.7745966692)^2/16} + (0.8888888889)e^{-(5)^2/16} + (0.5555555556)e^{-(5-0.7745966692)^2/16}\Big]$$

$$= 0.1093642$$

Maple: $\int_1^{1.5} e^{-x^2}\,dx = 0.1093642608$

$$\cong 0.1093643$$